



ICAMS Seminar

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Monday, July 11, 4:30 p.m. ICAMS Seminar room UHW 11/1102

Towards knowledge based material selection and - design

Combinatorial techniques are well established in pharmaceutical research for rapid screening and assessment of drugs. During the last decade combinatorial techniques were also used in materials science searching for new materials with attractive magnetic, ferroelectric, and catalytic properties. The assessment of structural materials has also been reported.

The combination of modern electronic structure calculations with the highly efficient combinatorial thin film composition-spread method constitutes an effective tool for knowledge based material selection and -design. Examples discussed in this paper include nanolaminates[1,2], hard coatings[2-3] solid lubricants[4] and thermoelectric materials[5] as well as Fe-Mn alloys[6,7].

[1] D.P. Sigumonrong, J. Zhang, Y. Zhou, D. Music, J.M. Schneider, Synthesis and elastic properties of V₂AlC thin films by magnetron sputtering from elemental targets, *J.Phys. D: Appl.Phys.* 42, 185408 (2009)

[2] Ahmed Abdulkadhim, Tetsuya Takahashi, Denis Music and Jochen M. Schneider, Phase evolution of magnetron sputtered TiC_x/Al (0.4 ≤ x ≤ 1.2) bilayer thin films upon annealing, accepted in *Acta Materialia* (2011)

[2] H. Kölpin, D. Music, G. Henkelmann, J. Emmerlich, F. Munnik, J.M. Schneider, Phase stability of AlYB₁₄ sputtered thin films, *J.Phys.: Condens. Matter* 21, 355006 (2009)

[3] J. Emmerlich, D. Music, M. Braun, P. Fayek, F. Munnik, J.M. Schneider, A proposal for an unusually stiff and moderately ductile hard coating material: Mo₂BC, *J.Phys. D: Appl.Phys.* 42, 185406 (2009)

[4] T. Reeswinkel, D. Music, and J.M. Schneider, Coulomb-potential-dependent decohesion of Magnéli phases, *Journal of Physics: Condensed Matter* 22 (29) (2010) 292203.

[5] D. Music, F. H.-U. Basse, and J. M. Schneider, Quantum mechanically guided design of transition metal alloyed RuO₂ nanorods, *Crystal Growth & Design* 10, 4531 (2010)

[6] T. Gebhardt, D. Music, M. Ekholm, I.A. Abrikosov, J. von Appen, R. Dronskowski, D. Wagner, J. Mayer, and J.M. Schneider, Influence of chemical composition and magnetic effects on the elastic properties of fcc Fe-Mn alloys, *Acta Materialia* 59 (4) (2011) 1493-1501.[7] T. Gebhardt, D. Music, D. Kossmann, M. Ekholm, I.A. Abrikosov, L. Vitos, and J.M. Schneider,

Elastic properties of fcc Fe-Mn-X (X = Al, Si) alloys studied by theory and experiment, *Acta Materialia* 59 (8) (2011) 3145-3155.

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